

Ethyl hexanoate
123-66-0 | DTXSID3021980

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 2.67

Global applicability domain: Inside

Local applicability domain index: 6.84e-01

Confidence level: 7.98e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Pentyl acetate</div> <div>Measured: 2.30</div> <div>Predicted: 2.27</div>	<div>Image not found</div> <div>3-Methylbutyl acetate</div> <div>Measured: 2.25</div> <div>Predicted: 2.20</div>	<div>Image not found</div> <div>Isobutyl methacrylate</div> <div>Measured: 2.66</div> <div>Predicted: 2.58</div>
<div>Image not found</div> <div>Heptyl acetate</div> <div>Measured: 3.46</div> <div>Predicted: 3.40</div>	<div>Image not found</div> <div>Butyl methacrylate</div> <div>Measured: 2.88</div> <div>Predicted: 2.66</div>	